Propofol - Compound Summary (CID 4943)

ASN1 XML SDF

An intravenous anesthetic agent which has the advantage of a very rapid onset after infusion or bolus injection plus a very short recovery period of a couple of minutes. (From Smith and Reynard, Textbook of Pharmacology, 1992, 1st ed, p206). Propofol has been used as ANTICONVULSANTS and ANTIEMETICS.

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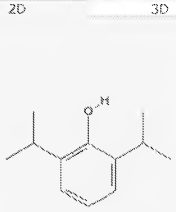
» Structure & Quick Link Bar

2D 3D



Ketcher PC3D Viewer Download

Compound ID	4943	
Molecular Weight	178.27072 [g/mol]	
Molecular Formula	$C_{12}H_{18}O$	
XLogP3	3.8	
H-Bond Donor	1	
H-Bond Acceptor	1	

BioMedical Annotation: (Total:1)

Propofol

Medication Information

Diprivan [General Injectables & Vaccines, Inc]
For IV Administration OnlyRx OnlyStrict aseptic technique must always be maintained during handling. Diprivan Injectable Emulsion is a single-use parenteral product which contains 0.005% disodium edetate to inhibit the rate of growth of more ...

Description	Clinical Pharmacology	Indication & Usage
Contraindications	Warnings	Precautions
Adverse Reactions	Overdosage	Dosage & Administration
How Supplied		

Diprivan Injectable Emulsion, USP [APP

Links

Protein Structure (3)
PubMed (29)
Gene (389)
Taxonomy (5)
NLM Toxicology Link

Chemical Structure Search
BioActivity Summary:
This Compound
with Similar Compounds

Related Compounds:
Same, Connectivity: 4 Links

Similar Compounds: 2137 Links
Similar Conformers: 1267 Links
View Conformers

Substances:
All: 189 Links
Same structure: 77 Links

Pharmaceuticals, LLC]

Mixture: 112 Links

Diprivan Injectable Emulstion, USP [APP Pharmaceuticals, LLC]

DIPRIVAN [AstraZeneca Pharmaceuticals LP]

PROPOFOL INJECTABLE EMULSION 1% [Bedford Laboratories]

PROPOFOL Injectable Emulsion 1% [Hospira, Inc.]

Propofol Injectable Emulsion 1% [Teva Parenteral Medicines, Inc.]

Propofol Injectable Emulsion, USP [APP Pharmaceuticals, LLC]

Propofol Injectable Emulsion, USP [APP Pharmaceuticals, LLC]

Propofol Injectable Emulsion, USP [APP Pharmaceuticals, LLC]

Propofol Injectable Emulsion, USP [APP Pharmaceuticals, LLC]

Pharmacological Action

Hypnotics and Sedatives - Drugs used to induce drowsiness or sleep or to reduce psychological excitement or anxiety.

Anesthetics, Intravenous - Ultrashort-acting anesthetics that are used for induction. Loss of consciousness is rapid and induction is pleasant, but there is no muscle ...

Pharmacological Classification

Chemical Actions and Uses
- Pharmacologic Actions
  - Physiological Effects of Drugs
    - Central Nervous System Depressants
      - Anesthetics
        - Anesthetics, General
          - **Anesthetics, Intravenous**
        - **Hypnotics and Sedatives**
      - **Hypnotics and Sedatives**
  - Therapeutic Uses
    - Central Nervous System Agents
      - Central Nervous System Depressants
        - Anesthetics
          - Anesthetics, General
            - **Anesthetics, Intravenous**
        - **Hypnotics and Sedatives**
      - **Hypnotics and Sedatives**

Chemical Classification

Organic Chemicals
Phenols
Propofol

Safety and Toxicology

HSDB - Peer-reviewed summary of toxicity and biomedical effects

CCRIS - Carcinogenicity, tumor promotion, tumor inhibition, and mutagenicity tests

EINECS - European Inventory of Existing Commercial Chemical Substances

TOXLINE - Citations to the toxicological literature

LactMed - Information on chemicals that breastfeeding mothers may be exposed

ClinicalTrials.gov - Registry of federal and private clinical trials

Literature Choose by Subheadings:

administration and dosage	adverse effects	agonists
analogs and derivatives	analysis	antagonists and inhibitors
blood	cerebrospinal fluid	chemical synthesis
chemistry	classification	contraindications
diagnostic use	economics	history
immunology	isolation and purification	metabolism
pharmacokinetics	pharmacology	poisoning
standards	supply and distribution	therapeutic use
toxicity	urine	

Literature Keyword Mining Tool

BioAssay Results:

Tested in BioAssays: All: 447 Active: 6 Inactive: 364
BioActivity Summary: This Compound with Similar Compounds

AID: 119873 **Source:** ChEMBL DataTable
Speed of induction of analgesia in mice was determined; I = immediate, <10 s

AID: 109886 **Source:** ChEMBL DataTable
Duration of analgesic action in mice was determined; B = brief, < 5 min

AID: 1195 **Source:** EPA DSSTox DataTable
DSSTox (FDAMDD) FDA Maximum (Recommended) Daily Dose Database

AID: 590 **Source:** NCGC DataTable
qHTS Assay for Spectroscopic Profiling in A350 Spectral Region

more ...

Protein Structures: (Total: 2)

MMDB ID: 75300 **PDB ID:** 3F33
Apoferritin: Complex With Propofol
Taxonomy: Equus caballus

MMDB ID: 15377 **PDB ID:** 1E7A
Crystal Structure Of Human Serum Albumin Complexed With The General Anesthetic Propofol
Taxonomy: Homo sapiens

Depositor-Supplied Synonyms: (Total: 126)

Display: Next 10 | All | Sort: Weight

propofol
Diprivan
Disoprofol
Disoprivan
Diisopropylphenol
2,6-DIISOPROPYLPHENOL
Propofolum
Dipravan
Fresofol
Rapinovet

Properties Computed from Structure:

Molecular Weight	178.27072 [g/mol]
Molecular Formula	$C_{12}H_{18}O$
XLogP3	3.8
H-Bond Donor	1

H-Bond Acceptor	1
Rotatable Bond Count	2
Tautomer Count	2
Exact Mass	178.135765
Monoisotopic Mass	178.135765
Topological Polar Surface Area	20.2
Heavy Atom Count	13
Formal Charge	0
Complexity	135
Isotope Atom Count	0
Defined Atom StereoCenter Count	0
Undefined Atom StereoCenter Count	0
Defined Bond StereoCenter Count	0
Undefined Bond StereoCenter Count	0
Covalently-Bonded Unit Count	1

Descriptors Computed from Structure:

IUPAC Name: 2,6-di(propan-2-yl)phenol
Canonical SMILES: CC(C)C1=C(C(=CC=C1)C(C)C)O
InChI: InChI=1S/C12H18O
/c1-8(2)10-6-5-7-11(9(3)4)12(10)13/h5-9,13H,1-4H3
InChIKey: OLBCVFGFOZPWHH-UHFFFAOYSA-N

Compound Information:

CID 4943
Create Date: 2005-03-25

Related Compounds:
Same, Connectivity: 4 Links

Similar Compounds: 2137 Links
Similar Conformers: 1267 Links View Conformers

Substance Information:

Substances:
All: 189 Links
Same structure: 77 Links
Mixture: 112 Links

Category: [for same structure substances]
Biological Properties: 32 Links
BIDD (1)
SID 93166594 - External ID: BIDD:GT0436
ChEBI (1)
SID 26697200 - External ID: CHEBI:44915
ChemBank (10)
ChemSpider (6)
Circadian Research, Kay Laboratory, University of California at San Diego (UCSD) (1)
SID 92303746 - External ID: D126608
Comparative Toxicogenomics Database (1)

SID 53788803 - External ID: D015742
DiscoveryGate (1)
SID 8153049 - External ID: 4943
DrugBank (1)
SID 46504991 - External ID: DB00818
DTP/NCI (1)
SID 71265 - External ID: 5105
ICCB-Longwood/NSRB Screening Facility, Harvard Medical School (3)
SID 92125828 - External ID: HMS1570L04
SID 92308977 - External ID: HMS2089O21
SID 92308180 - External ID: HMS2094E17
LeadScope (1)
SID 49855158 - External ID: LS-996
NextBio (1)
SID 80426669 - External ID: 4943
NIAID (1)
SID 219945 - External ID: 123996
NovoSeek (1)
SID 57322542 - External ID: 4943
Southern Research Institute (1)
SID 49699215 - External ID: AB00513968
xPharm (1)
SID 7980416 - External ID: 9305

Chemical Reactions: 8 Links
ChemSpider (6)
Comparative Toxicogenomics Database (1)
SID 53788803 - External ID: D015742
KUMGM (1)
SID 7984535 - External ID: ghl.PD_Mitscher_leg0.558

Journal Publishers: 2 Links
Prous Science Drugs of the Future (1)
SID 12012653 - External ID: 90057
Thomson Pharma (1)
SID 14772701 - External ID: 00003209

Metabolic Pathways: 4 Links
BioCyc (1)
SID 85256986 - External ID: CPD-11437
Comparative Toxicogenomics Database (1)
SID 53788803 - External ID: D015742
KEGG (2)
SID 9726 - External ID: C07523
SID 7847615 - External ID: D00549

NIH Molecular Libraries: 14 Links
Broad Institute (1)
SID 85788322 - External ID: BRD-K82255054-001-03-5
Emory University Molecular Libraries Screening Center (2)
SID 17405000 - External ID: EU-0100437
SID 26612728 - External ID: SPECTRUM1505022
NCGC (10)
University of Pittsburgh Molecular Library Screening Center (1)
SID 53777543 - External ID: 391

NIH Substance Repository: 2 Links

MLSMR (2)
SID 47193694 - External ID: MLS001056348
SID 85148728 - External ID: MLS002454360

Physical Properties: 13 Links
ChemExper Chemical Directory (1)
SID 3132933 - External ID: HklH@@RYfVya`Hbj@@@
ChemSpider (6)
DrugBank (1)
SID 46504991 - External ID: DB00818
MP Biomedicals (2)
SID 85088964 - External ID: 193707
SID 51074363 - External ID: 204044
NIST (1)
SID 10427917 - External ID: 1803667406
NIST Chemistry WebBook (1)
SID 10513227 - External ID: 1803667406
NMRShiftDB (1)
SID 8001758 - External ID: 20040435

Protein 3D Structures: 3 Links
MMDB (2)
SID 838001 - External ID: 15377.3
SID 81087128 - External ID: 75300.8
SMID (1)
SID 7889810 - External ID: PFL

Substance Vendors: 13 Links
Ambinter (1)
SID 48505627 - External ID: ST5405911
ChemExper Chemical Directory (1)
SID 3132933 - External ID: HklH@@RYfVya`Hbj@@@
ChemSynthesis (1)
SID 56289300 - External ID: 19324
Hangzhou APIChem Technology (1)
SID 92716688 - External ID: AC-2038
IS Chemical Technology (1)
SID 81042045 - External ID: S01-0189
Jamson Pharmachem Technology (1)
SID 96022658 - External ID: Jsp004266
MolPort (1)
SID 88837501 - External ID: MolPort-001-794-517
MP Biomedicals (2)
SID 85088964 - External ID: 193707
SID 51074363 - External ID: 204044
Sigma-Aldrich (2)
SID 24278001 - External ID: D126608_ALDRICH
SID 24902022 - External ID: W505102_ALDRICH
TCI (Tokyo Chemical Industry) (1)
SID 87567266 - External ID: D0617
ZINC (1)
SID 12055958 - External ID: ZINC00968303

Theoretical Properties: 9 Links
ChemDB (1)
SID 5371511 - External ID: 3968273
ChemSpider (6)
DrugBank (1)
SID 46504991 - External ID: DB00818
ZINC (1)

SID 12055958 - External ID: ZINC00968303

Toxicology: 4 Links
ChemIDplus (1)
SID 159631 - External ID: 002078548
Comparative Toxicogenomics Database (1)
SID 53788803 - External ID: D015742
EPA DSSTox (2)
SID 48416482 - External ID: 23523
SID 48424532 - External ID: 32895

ASN1 XML SDF